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(FILE 'HOME' ENTERED AT 15:35:39 ON 17 JUN 2003)

FILE 'CAPLUS' ENTERED AT 15:36:20 ON 17 JUN 2003
L1 260 S ((THREE (2W) DIMENSION?) OR 3D) AND (ROOT MEAN SQUARE) AND (P
L2 188 S (((THREE (2W) DIMENSION?) OR 3D) (W) STRUCTURE) AND (ROOT ME
L3 0 S L2 AND PATENT/DT
L4 188 SORT L2 PY

=> d bib,abs 5,9,12,22,35,45,53,55,60

L4 ANSWER 5 OF 188 CAPLUS COPYRIGHT 2003 ACS
AN 1988:2314 CAPLUS
DN 108:2314
TI Refined **three-dimensional structures** of two cyanobacterial C-phycocyanins at 2.1 and 2.5 .ANG. resolution. A common principle of phycobilin-**protein** interaction
AU Schirmer, Tilman; Bode, Wolfram; Huber, Robert
CS Max-Planck-Inst. Biochem., Martinsried, D-8033, Fed. Rep. Ger.
SO Journal of Molecular Biology (1987), 196(3), 677-95
CODEN: JMOBAK; ISSN: 0022-2836
DT Journal
LA English
AB The crystal structure of the light-harvesting **protein-pigment** complex C-phycocyanin (C-PC) from Mastigocladus laminosus (at 2.1-.ANG. resoln.) has been refined by energy-restrained least-squares methods to a conventional R-factor of 21.7%. In the same way, the crystal structure of C-PC from Agmenellum quadruplicatum has been refined further (2.5 .ANG., R = 18.4%); pyrrole rings C and D of the chromophore at position A84 have been cor. with respect to the previously reported structure. The 2 C-PC structures are very similar, 213 C.alpha. positions have a **root-mean-squares** deviation of 0.49 .ANG.. Polar and ionic side-chain interactions are discussed in detail, and the 2 subunits of C-PC from M. laminosus are compared to each other. All 3 chromophores are completely defined and their tetrapyrroles exhibit very similar geometry. The structure of a C-PC chromophore resembles a cleaved porphyrin which has been twisted .apprx.180.degree. around the C-5-C6 and C-14-C-15 bonds. Accordingly, th configuration/conformation of the chromophores is Z-anti, Z-syn, Z-anti (with the exception of the configuration of C-15 of chromophore B155, which is almost midway between Z- and E-). The 3 chromophores interact similarly with the **protein**. They arch around aspartate residues (A87, B87, and B39), and the N atoms of pyrroles B and C are within H-bonding distance of 1 of the carboxylate O atoms. Most of the propionic side chains of the chromophores form salt bridges with arginine and lysine residues. The updated relative chromophore distances and orientations confirm the conclusion that hexameric aggregates are probably the basic functional units, and that interhexameric energy transfer takes place preferentially via the central B84 chromophores.

L4 ANSWER 9 OF 188 CAPLUS COPYRIGHT 2003 ACS
AN 1988:488406 CAPLUS
DN 109:88406
TI **Three-dimensional structure** of acyl carrier **protein** in solution determined by nuclear magnetic resonance and the combined use of dynamical simulated annealing and distance geometry
AU Holak, Tadeusz A.; Nilges, Michael; Prestegard, James H.; Gronenborn, Angela M.; Clore, G. Marius
CS Max-Planck-Inst. Biochem., Martinsried, Fed. Rep. Ger.
SO European Journal of Biochemistry (1988), 175(1), 9-15
CODEN: EJBCAI; ISSN: 0014-2956
DT Journal
LA English

AB The soln. conformation of acyl carrier protein of Escherichia coli (77 residues) was detd. on the basis of 423 interproton-distance restraints and 32 H-bonding restraints derived from NMR measurements. A total of 9 structures were computed using a hybrid approach combining metric matrix distance geometry and dynamic simulated annealing. The polypeptide fold was well defined with an av. backbone at root-mean-square difference of 0.20 nm between the final 9 converged structures and the mean structure obtained by averaging their coordinates. The principal structural motif was composed of 3 helices: 1 (residues 3-12), 2 (residues 37-47), and 4 (residues 65-75) which lined a hydrophobic cavity. Helices 2 and 4 were approx. parallel to each other and anti-parallel at an angle of .apprx.150.degree. to helix 1. The smaller helix 3 (residues 56-63) was at an angle of .apprx.100.degree. to helix 4.

L4 ANSWER 12 OF 188 CAPLUS COPYRIGHT 2003 ACS
AN 1990:51165 CAPLUS

AN 1990:51163 CAPLUS
DN 113:51165

DN 112:51165
TI Datenw...
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11 Determination of the complete three-dimensional
structure of the trypsin inhibitor from squash seeds in aqueous
solution by nuclear magnetic resonance and a combination of distance
geometry and dynamical simulated annealing

AU Holak, T. A.; Gondol, D.; Otlewski, J.; Wilusz, T.

CS Max-Planck-Inst. Biochem. Martinsried D-8033 Fed. Rep. G

SO Journal of Molecular Biology (1988) 210 (3): 625-636

JOURNAL OF MOLECULAR BIOLOGY (1989), 210(3), 635-48
CODEN: JMOBAK ISSN: 0022-2833

DT CODEN: UMOBAR; ISSN: 0022-2836

Journal
Editor

LA English

AB The complete 3-dimensional structure of the trypsin inhibitor from seeds of the squash *Cucurbita maxima* in aq. soln. was detd. on the basis of 324 interproton distance constraints, 80 non-nuclear Overhauser effect distances, and 22 H-binding constraints, supplemented by 27 .PHI. backbone angle constraints derived from NMR measurements. The NMR input data were converted to the distance constraints in a semiquant. manner after a sequence specific assignment of 1H spectra was obtained using 2-dimensional NMR techniques. Stereospecific assignments were obtained for 17 of the 48 prochiral centers of the squash trypsin inhibitor using the floating chirality assignment introduced at the dynamical simulated annealing stage of the calcns. A total of 34 structures calcd. by a hybrid distance geometry-dynamical simulated annealing method exhibit well-defined positions for both backbone and side-chain atoms. The av. at. **root-mean-square** difference between the individual structures and the minimized mean structure is 0.35 .ANG. for the backbone atoms and 0.89 .ANG. for all heavy atoms. The precision of the structure detn. is discussed and correlated to the exptl. input data.

L4 ANSWER 22 OF 188 CAPLUS COPYRIGHT 2003 ACS
AN 1991:553806 CAPLUS

DN 115:153806

BN 119:15386
TI Similarity of the three-dimensional structures
of actin and the ATPase fragment of a 70-kDa heat shock cognate
protein

AU Flaherty, Kevin M.; McKay, David B.; Kabsch, Wolfgang; Holmes, Kenneth C
CS Sch. Med., Univ. of Michigan

CS Sch. Med., Stanford Univ., Stanford, CA, 94305-5400, USA

SO Proceedings of the National Academy of Sciences of the United States of America

America (1991), 88(11), 5041-5

CODEN: PNASA6; ISSN: 0027-8424

DT Journal

LA English

EN English
AB Although

AB Although there is very little sequence identity between the 2 proteins, the structures of rabbit skeletal muscle actin (375-amino acid residues) and the 44-kDa ATPase fragment of the bovine 70-kDa heat shock cognate proteins (HSC70; 386 residues) are very similar. The .alpha.-C positions of 241 pairs of amino acid residues

that are structurally equiv. within the 2 proteins can be superimposed with a root-mean-square difference in distance of 2.3 .ANG.; of these, 39 residues are identical, and 56 are conservative substitutions. In addn., the conformations of ADP are very similar in both proteins. A local sequence fingerprint, which may be diagnostic of the adenine nucleotide beta-phosphate-binding pocket, has been derived. The fingerprint identifies members of the glycerol kinase family as candidates likely to have a similar structure in their nucleotide-binding domains. The structural differences between the 2 mols. mainly occur in loop regions of actin known to be involved in interactions with other monomers in the actin filament or in the binding of myosin; the corresponding regions in heat shock proteins may have functions that are as yet undetd. Placing the Ca²⁺-ATP of actin on the ATPase fragment structure suggests Asp-206 (corresponding to His-161 of actin) as a candidate proton acceptor for the ATPase reaction.

L4 ANSWER 35 OF 188 CAPLUS COPYRIGHT 2003 ACS
AN 1993:51863 CAPLUS
DN 118:51863
TI Comparative molecular modeling and crystallization of P-30 protein : A novel antitumor protein of Rana pipiens oocytes and early embryos
AU Mosimann, Steven C.; Johns, Kathy L.; Ardel, Wojciech; Mikulski, Stanislaw M.; Shogen, Kuslima; James, Michael N. G.
CS Dep. Biochem., Univ. Alberta, Edmonton, AB, T6G 2H7, Can.
SO Proteins: Structure, Function, and Genetics (1992), 14(3), 392-400
CODEN: PSFGEY; ISSN: 0887-3585
DT Journal
LA English
AB The P-30 protein (Onconase) of R. pipiens oocytes and early embryos is homologous to members of the pancreatic RNase superfamily and exhibits an antitumor activity in vitro and in vivo. It appears that the ribonucleolytic activity of P-30 protein may be required for its antitumor effects. A comparative mol. model of P-30 protein has been constructed based upon the known three-dimensional structure of bovine pancreatic RNase A in order to provide structural information. Functionally, these enzymes hydrolyze oligoribonucleotides to pyrimidine-3'-phosphate monoesters and 5'-OH ribonucleotides. In the modeling procedure, automated sequence alignments were revised based upon the inspection of the RNase A structure before the amino acids of the P-30 protein were assigned to the coordinates of the RNase A template. The inevitable intermol. steric clashes that result were relieved on an interactive graphics device through the adjustment of side chain torsion angles. This process was followed by energy minimization of the model, which served to optimize stereochem. geometry and to relieve any remaining unacceptably close contacts. The resulting model retains the essential features of RNase A as sequence insertions and deletions are almost exclusively found in exposed surface loops. The all atom superposition of active site residues of the P-30 protein model and an identically minimized RNase A structure has a root mean square deviation of 0.52 .ANG.. Though tentative, the model is consistent with a pyrimidine specificity. Further, the model suggests Lys9 (P-30 protein) can donate a hydrogen bond to the active site phosphate, whereas it is unlikely that P-30 protein binds the 3'-ribonucleotide in a fashion similar to RNase A. P-30 protein has been crystd. in an orthorhombic space group, P212121, with unit cell dimensions, a = 40.76, b = 69.77, and c = 32.54 .ANG.. The crystals grow as small rosettes from an ammonium sulfate soln. at pH 4.5.

L4 ANSWER 45 OF 188 CAPLUS COPYRIGHT 2003 ACS
AN 1992:168903 CAPLUS
DN 116:168903

TI Three-dimensional structure of
Gln25-ribonuclease T1 at 1.84-.ANG. resolution: structural variations at
the base recognition and catalytic sites
AU Arni, Raghuvir K.; Pal, Gour P.; Ravichandran, K. G.; Tulinsky, Alexander;
Walz, Frederick G., Jr.; Metcalf, Peter
CS Eur. Mol. Biol., Heidelberg, D-6900, Germany
SO Biochemistry (1992), 31(12), 3126-35
CODEN: BICAW; ISSN: 0006-2960
DT Journal
LA English
AB The structure of the Gln25 variant of RNase T1 (RNase T1) crystd. at pH 7
and at high ionic strength has been solved by mol. replacement using the
coordinates of the Lys25-RNase T1/2'-guanylic acid (2'GMP) complex at pH 5
(Arni, R., et al., 1988) and refined by energy minimization and
stereochem. restrained least-squares minimization to a crystallog.
R-factor of 14.4% at 1.84 .ANG. resoln. The asym. unit contains three
mols. and the final model consists of 2302 protein atoms, 3
sulfates (at the catalytic sites) and 179 solvent water mols. The estd.
root mean square (rms) error in the
coordinates is 0.15 .ANG., and the rms deviation from ideality is 0.018
.ANG. for bond lengths and 1.8.degree. for bond angles. Significant
differences are obsd. between the three mols. in the asym. unit at the
base recognition and catalytic sites.

L4 ANSWER 53 OF 188 CAPLUS COPYRIGHT 2003 ACS
AN 1993:665872 CAPLUS
DN 119:265872
TI Conformational classification of short backbone fragments in globular
proteins and its use for coding backbone conformations
AU Takahashi, Katsutoshi; Go, Nobuhiro
CS Fac. Sci., Kyoto Univ., Kyoto, 606, Japan
SO Biophysical Chemistry (1993), 47(2), 163-78
CODEN: BICIAZ; ISSN: 0301-4622
DT Journal
LA English
AB An objective and systematic method of coding backbone conformations of
proteins is developed. For this purpose the polypeptide
backbone is regarded to consist of two types of overlapping structural
units, viz. a (.phi., .psi.) fragment (C_i.alpha.-C'_iO-N-C_{i+1}.alpha.-C'_{i+1}O-N-
C_{i+2}.alpha.), and a (.psi., .phi.) fragment (N-C_i.alpha.-C'_iO-N-C_{i+1}.alpha.-
C'). By means of the principal component anal., these (.phi., .psi.) and
(.psi., .phi.) fragments are found to form five and six distinct clusters
in resp. high-dimensional conformational space with only a small no. of
exceptional unclassified fragments. Boundaries of clusters are defined by
multi-dimensional ellipsoids. This classification of conformations of
short backbone fragments is used to code protein backbone
three-dimensional structures. In particular,
conformations of peptide fragments consisting of four or six residues are
coded and analyzed in detail. This structural code permits the
recognition of features of protein backbone structures that are
not retained in the usual secondary structural representation based on
patterns of backbone hydrogen bonds, e.g., various types of four-residue
turns. The similarity index, based on the no. of different one-letter
codes in a pair of structural codes, is a powerful measure of
conformational similarity. When combined with another similarity measure,
at. **root-mean-square** distance, accurate
similarity between a pair of conformations of fragments can be detected.

L4 ANSWER 55 OF 188 CAPLUS COPYRIGHT 2003 ACS
AN 1993:620791 CAPLUS
DN 119:220791
TI Protein modeling using a chimera reference protein
derived from exons
AU Kajihara, Akiro; Komooka, Hitoshi; Kamiya, Kenshu; Umeyama, Hideaki

CS Sch. Pharm. Sci., Kitasato Univ., Tokyo, 108, Japan
SO Protein Engineering (1993), 6(6), 615-20
CODEN: PRENE9; ISSN: 0269-2139
DT Journal
LA English
AB Bovine pancreatic .beta.-trypsin (PDB ID-code: 1TPO) which is registered in the Brookhaven Protein Data Bank (PDB) consists of four exons. The results of homol. searches for each exon in the PDB showed that homologous proteins were tonin (PDB ID-code: 1TON), rat mast cell protease (PDB ID-code: 3RP2-A), kallikrein A (PDB ID-code: 2PKA-B) and kallikrein A (2PKA-B), resp. Thus, for the three-dimensional structure prediction of 1TPO, a chimera protein was constructed from the three proteins mentioned above and the 3-D structure prediction was performed using this chimera ref. protein. The modeled structure of 1TPO was energetically optimized by mol. mechanics and mol. dynamics simulation and was compared with its x-ray crystal structure registered in the PDB. The root mean square deviations (r.m.s.d.) of main chain atoms and the neighboring active site (5 .ANG. sphere from His57, Asp102 and Ser195) between the modeled structure and the x-ray structure were 1.66 and 0.94 .ANG., resp. Porcine pancreatic elastase (PDB ID-CODE: 3EST) which is registered in the PDB was used as the ref. protein and the modeled structure from 3EST was also compared with the x-ray data. The r.m.s.d. of main chain atoms and that of the active site were 2.14 and 1.18 .ANG., resp. These results clearly support the propriety of this method using the chimera ref. protein.

L4 ANSWER 60 OF 188 CAPLUS COPYRIGHT 2003 ACS
AN 1993:555384 CAPLUS
DN 119:155384
TI Structural consequences of reductive methylation of lysine residues in hen egg white lysozyme: An x-ray analysis at 1.8-.ANG. resolution
AU Rypniewski, Wojciech R.; Holden, Hazel M.; Rayment, Ivan
CS EMBL, Hamburg, 2000/52, Germany
SO Biochemistry (1993), 32(37), 9851-8
CODEN: BICHAW; ISSN: 0006-2960
DT Journal
LA English
AB Chem. modification of proteins has been and continues to be an important biochem. tool for the study of protein structure and function. One such type of approach has been the reductive methylation of lysine residues. In order to address the consequences of such methylation on the crystn. and structural properties of a protein, the three-dimensional structure of hen egg white lysozyme in which all lysine residues have been alkylated has been detd. and refined to a nominal resoln. of 1.8 .ANG. and a crystallog. R factor of 17.3%. Crystals used in the investigation were grown from 1.5-1.8 M MgSO₄ and 50 mM Tris at pH 8.0 and belonged to the space group P212121 with unit cell dimensions of a = 30.6 .ANG., b = 56.3 .ANG., c = 73.2 .ANG., and one mol. per asym. unit. It was not possible to grow crystals of the modified lysozyme under the conditions normally employed for the hen egg white protein. Overall, the three-dimensional structures of the native lysozyme and the modified protein are very similar with only two surface loops differing to any significant extent. Specifically, the positions of the alpha-carbons for these two forms of the protein, excluding the surface loops, superimpose with a root-mean-square value of 0.40 .ANG.. The magnitude of the structural changes obsd. between the modified and unmodified forms of lysozyme is similar to that seen when an identical protein structure is solved in two different cryst. lattices. Consequently, the methylation of lysine residues results in very little structural perturbations but can produce enormous effects of the crystn. properties of a protein. As described here, this technique was absolutely crit. for obtaining X-ray

quality crystals of myosin subfragment I and thus may prove to be valuable
in the crystn. of other **proteins** that have so far resisted
forming ordered arrays.